Avoided Quantum Criticality near Optimally Doped High Temperature Superconductors

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We study the crossover from the underdoped to the overdoped regime in the t-J model. The underdoped regime is dominated by the superexchange interaction, locking the spins into singlets which weakly perturbe coherent charge carriers. In the overdoped, large carrier concentration regime, the Kondo effect dominates resulting in spin-charge composite quasiparticles which are also coherent. Separating these two Fermi liquid regimes, there is a critical doping where superexchange and Kondo interaction balance each other, bringing the system close to a local quantum critical point near the point of maximal superconducting transition temperature. At this point, particle hole symmetry is dynamically restored and physical quantities such as the optical conductivity, exhibit power law behaviour at intermediate frequencies as observed experimentally. Quantum criticality is avoided by the onset of superconductivity.

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The high temperature superconductors have a normal state which is not well described by the standard theory of metals [1]. Several anomalies are well established experimentally: a) The normal state close to the doping level with the highest transition temperature is highly incoherent and does not fit the standard Fermi liquid picture, b) at small doping the normal state has a pseudogap, c) the optimally doped regime exhibits anomalous power laws in transport quantities and in the optical conductivity in an intermediate frequency range. This observation has lead to the suggestion that the superconducting dome covers a critical point [2], d) The superconducting state not only exhibits coherent Bogolubov quasiparticles and charge collective modes, but also a very sharp spin mode or "40 meV resonance". The role of this mode as well as of the putative quantum critical fluctuations in a fundamental theory of cuprate supercondcutivity are important issues.

In this letter we present a coherent account of these observations based on a Cluster Dynamical Mean Field Theory analysis of the t-J model. This approach allows us to access the regime of intermediate temperatures in the doping regime between underdoped to overdoped system. In addition, the approach is formulated in terms of pseudoparticles, representing collective excitations of the system in an enlarged Hilbert space. This formulation provides a clear interpretation of the numerical results, providing a transparent physical interpretation.

We start from the the t-J model which was proposed by P.W. Anderson as a minimal model to describe the cuprate superconductors

$$H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2}\sum_{ij} \mathbf{S}_i \mathbf{S}_j. \qquad (1)$$

It contains two terms; one describes the kinetic energy which delocalizes the holes introduced by doping, and a spin spin interaction. A constraint of no double occupancy must be enforced.

We used the extended Dynamical Cluster Approximation [3] combined with the slave particle approach [4] which have been very useful in the theory of strongly correlated electrons. The cluster approach maps the full many body problem, into a a set of local degrees of freedom (in this case a two by two plaquette) which are treated exactly and a bath which is treated self consistently.

The coupling of the cluster to the medium, which simulates the rest of the lattice, causes the cluster eigenstates to decay in time therefore their spectral functions carry nontrivial frequency dependence and important information about various physical processes such as the RKKY interactions, the Kondo effect and d-vawe superconductivity. To study the dynamics of the cluster states, we diagonalized the cluster, i.e., $H_{cluster}|m\rangle = E_m|m\rangle$, and assigned to each cluster eigenstate a pseudoparticle $|m\rangle = a^\dagger_m|0\rangle$. The original problem can be exactly expressed in terms of pseudoparticles a_m with the only non-quadratic term of the converted Hamiltonian being the hybridization between the cluster and the medium. This cubic hybridization term is taken into account by the self-consistent resummation of the non-crossing diagrams in the spirit of the well known Non-Crossing approximation to the Anderson impurity model. Since the Hilbert space of the new base of pseudoparticles accesses some non-physical states, one needs to project them out with the constraint expressing the completeness of the cluster eigenbasis. First we calculate the pseudoparticle self energies and the pseudoparticle Greens functions. Finally, physical observables like spectral function or susceptibilities can be calculated by a weighted sum of the convolution of the pseudoparticle spectral functions. The following matrix elements $(F^{\mathbf{K}\dagger})_{nm} = \langle n|c^\dagger_{\mathbf{K}}|m\rangle$ and $(\mathbf{S}_Q)_{nm} = \langle n|\mathbf{S}_Q|m\rangle$ give the bare weight of the electron

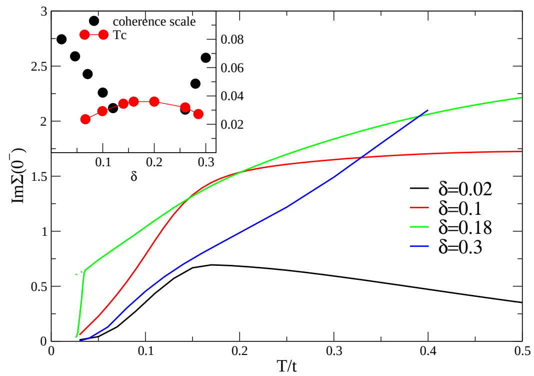

FIG. 1: The cluster $(\pi, 0)$ self-energy at zero frequency as a function of temperature for few doping levels. The inset shows the estimation of the coherent scale in the normal state of the t-J model (black dots) and transition temperature to superconducting state (red dots).

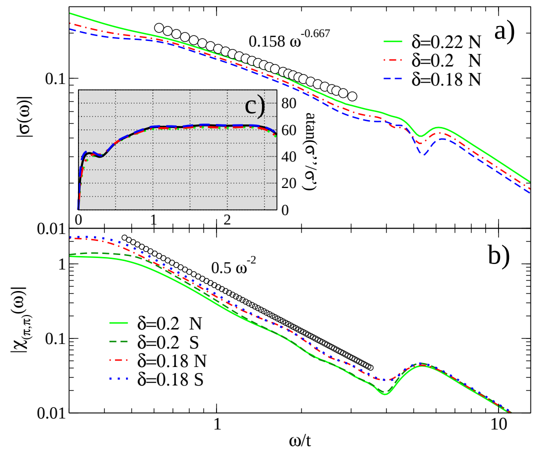

FIG. 2: a) The absolute value of complex optical conductivity $\sigma(\omega)$ is proportional to $\omega^{-2/3}$ in the intermediate frequency region for optimally doped system. b) The absolute value of the (π, π) spin sussceptibility is proportional to ω^{-2}. c) The angle, calculated as $\arctan(\mathrm{Im}(\sigma)/\mathrm{Re}(\sigma))$ is approximately $\pi/3$ since $\sigma(\omega) \sim (-i\omega)^{-2/3}$. In the legend, N stand for normal state and S for superconducting state.

spectra and the spin response in terms of pseudoparticles

$$G_{\mathbf{K}}(i\omega) = - \sum_{nmn'm'} (F^{\mathbf{K}})_{m'n'} C_{m'n'nm}(i\omega) (F^{\mathbf{K}\dagger})_{nm} \quad (2)$$

$$\chi^{\alpha\beta}_{\mathbf{Q}}(i\omega) = \sum_{nmn'm'} (S^{\alpha}_{\mathbf{Q}})_{m'n'} C_{m'n'nm}(i\omega) (S^{\beta}_{-\mathbf{Q}})_{nm} \quad (3)$$

with

$$C_{m'n'nm}(i\omega) = T \sum_{i\epsilon} G_{n'n}(i\epsilon) G_{mm'}(i\epsilon - i\omega) \quad (4)$$

Here $G_{\mathbf{K}}$, $G_{nn'}$ and $\chi_{\mathbf{Q}}$ are electron Green's function, pseudoparticle Green's function and spin susceptibility, respectively. This is the central equation of the approach, relating observables to the pseudoparticle spectral functions plotted in Fig. 4. More details of the method can be found in [5]. It has been shown that the cluster approach successfully describes many properties of the high temperature superconductors [3, 5, 6]. In this letter we show that it also unravels the origin of the apparent criticality observed near critical doping, and its elimination below the superconducting state.

Physically pseudoparticles represent coarsed grained versions of the important many body excitations including fermionic quasiparticles and bosonic collective modes. They have quantum numbers describing their spin, number of particles, (which divided by the cluster size, give the density), and a coarsed grained momentum. In momentum space, the course graining for the smallest cluster divides the Brillouin zone into four different regions, namely an inert patch around $(0, 0)$ point, the second patch centered around (π, π) being highly non-Fermi liquid like at small doping and finally $(\pi, 0)$ and $(0, \pi)$ regions which contain the Fermi surface of the model in the underdoped and slightly overdoped regime and are therefore most relevant for thermodynamical and transport properties.

The first indication for an underlying criticality near optimal doping comes from the evaluation of the electron scattering rate obtained from the imaginary part of the electron self-energy as a function of temperature for few different doping levels. As described in Fig. 1 both at large and small doping the scattering rate is small as expected for a Fermi liquid. Remarkably it becomes very large in the region near optimal doping when the critical temperature is maximal. The transition to the superconducting state severely reduces the scattering rate eliminating the traces of the underlying critical behaviour, hence the name avoided quantum criticality. A coherence scale, estimated from the scattering rate, is plotted in the inset of Fig. 1 and shows it tends to vanish close to the point of maximal superconducting transition temperature.

Additional evidence for the quantum criticality is the emergence of power-law behaviours of the response functions. As shown in Fig. 2, the optical conductivity has an approximate power law with an exponent $2/3$. The same powerlaw is realized in the one-electron self-energy while the spin susceptibility is proportional to $\chi_{\pi,\pi} \propto \omega^{-2}$ in the same frequency range. Experimentally, it was found that the optical conductivity is proportional to the $(-i\omega)^{-0.65}$ in the intermediate frequency regime [7].

Quantum criticality is avoided when the electrons condense forming d-wave pairs. The electron scattering rate is dramatically reduced (see Fig. 1) and a V-shaped gap opens in the local one-electron density of states. The particle-hole response at (π, π) is severely reduced for frequencies below the superconducting gap and a sharp resonance appears in the gap. A sharp resonance peak in the spin susceptibility was observed in bilayer cuprates

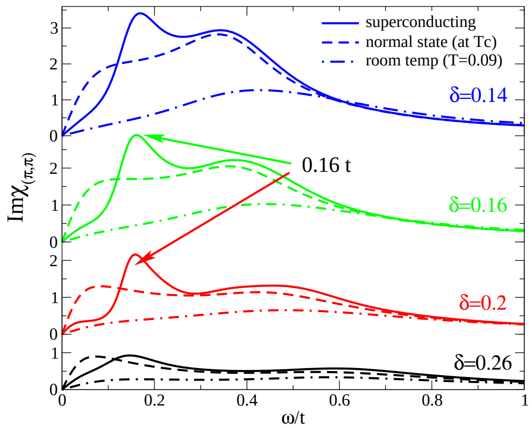

FIG. 3: The dynamical spin susceptibility at $\mathbf{q} = (\pi, \pi)$ for few different doping levels and three different temperatures: superconducting state, normal state at the transition temperature and at room temperature. The pronounced peak is formed in SC state at $0.16t \approx 48\,\mathrm{meV}$ and a broad peak in normal state is around $100 - 140\,\mathrm{meV}$. Susceptibility at normal temperture is much smaller and the peak moves to higher frequencies. The resonance is strongest at the optimally doped system. It disappears quickly in the overdoped site and somewhat more slowly in the underdoped side.

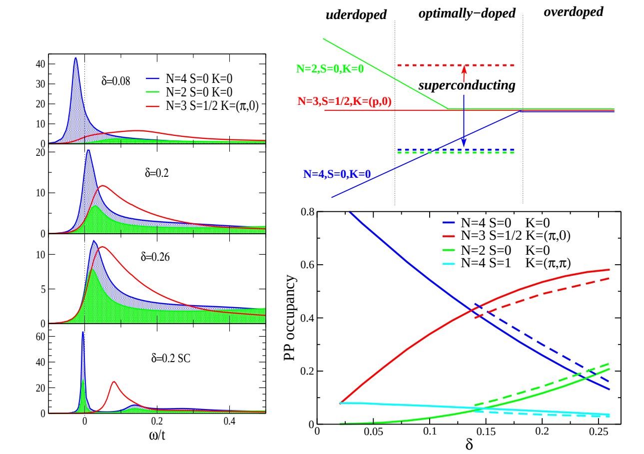

FIG. 4: left: Pseudoparticle spectral functions for the three most important pseudoparticles: ground states for N=4, N=3 and N=2 sectors. Right-top: Sketch of pseudoparticle treshold energies which can be interpreted as the effective many-body levels in normal and superconducting state. Right-bottom: Pseudoparticle occupancies versus doping for most important pseudoparticles. The full lines correspond to the normal state while the dashed lines correspond to the superconducting state.

YBCO and Bi2212 and in singe layer Tl2201. It scales with doping like $5T_c$ and does not depend on temperature.

Our method gives a pronounced peak in the (π, π) spin response at frequency $0.16t$ in the optimally doped regime, as shown in Fig. 3. The peak position is temperature independent and taking into account the maximal transition temperature in our model $T_{c-max} \sim 0.035t$ the resonance energy is $4.6T_c$ in good agreement with experiments.

In addition we see a broader peak around $0.35 - 0.45t$ extending to very high frequencies of order of $t \approx 300\,\mathrm{meV}$ which also gains some weight upon condensation and represents an important contribution to the exchange energy difference between superconducting and normal state. This exchange energy gives far the largest contribution to the condensation energy [5].

Our method averages the momentum dependence over $1/4$ of the Brillouin zone centered at (π, π) therefore it is reasonable to compare our results with the $\mathbf{q}$ integrated susceptibility from Ref. 8 where both the $35\,\mathrm{meV}$ resonant peak as well as broader peak around $75\,\mathrm{meV}$ extending up to $220\,\mathrm{meV}$ was observed.

Pseudoparticle interpretation: These results can be understood in terms of the evolution of the pseudoparticle spectral functions (spectral functions of the eigenstates of the plaquette) depicted in Fig. 4. Remarkably, out of the large number of pseudoparticles which are involved in our calculation (3^4) only four distinct pseudoparticles are very important, having the largest weight in the ground state and containing more than 95% of the spectral weight of the low energy correlation functions. Fig. 4a shows the evolution of the three most important pseudoparticle spectral functions from the underdoped to the overdoped regime.

Underdoped Regime: At small doping, the singlet state with one particle per site and zero momentum (N=4,S=0,K=0) (half filled singlet) dominates since it has far the lowest treshold energy, is very strongly peaked at the treshold energy, and has the largest occupancy as shown in Fig. 4c,. It describes a system locked in a short range singlet state as a consequence of the strong superexchange interaction. The electron spectral function descrbies the process of addition and removal of an electron from the system at frequency ω. It is dominated by convolution of two pseudoparticles with different cluster occupation N and N+1, or N-1 and with integral in convolution taken between zero and ω. The necessary condition for a peak of the one-particle spectral function at the Fermi level is that at least two pseudoparticle spectral functions share common threshold and are strongly peaked at the same threshold. Since the thresholds of the other pseudoparticles are significantly shifted with reference to the half filled singlet, a pseudogap results in the one particle spectra in the underdoped regime. This gap in threshold energies severely limits the possible decay processes of the electron resulting in a low electronic scattering rate.

The local picture of the overdoped regime: On the overdoped side, all three important pseudoparticles (half-filled singlet, doublet with one hole per plaquette and singlet with two holes per plaquette) have a power law

divergence at the same threshold frequency at zero temperature (Fig. 4a and Fig. 4b) which is a standard signature of the Kondo effect. Hence, the one particle spectral function develops the Kondo-Suhl resonance at the Fermi level since the convolution between the doublet and half-filled singlet (or N=2 singlet) state is large at low frequency. The one-particle spectral function is peaked slightly above the Fermi level. The underdoped regime is distinctively different since only the half-filled singlet state dominates while the doublet has very little spectral weight in the region of the singlet peak.

The Transition Region, Normal State: In the optimal doped regime, the Kondo effect and the superexchange compete giving rise to a regime with very large scattering rate and consequently a small coherence scale. Criticality is the result of the merging of the convergence of the thresholds of the pseudoparticles (See Fig 4) when going from the underdoped to the overdoped regime. Local criticality has been found in models of heavy fermion systems [9] and frustrated magnets [10].

Surprisingly this evolution is accompanied by a restoration of particle hole symmetry in the optimally doped regime. As shown in Fig. 4b the threshold of the N=2 cluster ground state and N=3 cluster ground state (doublet) merge first resulting in a Kondo-like contribution to the electron spectral function. This contribution is peaked above the Fermi level as usual for the simple Fermi-liquid state in less than half-filled one band model. The half-filled singlet however remains the lowest state in energy and still gives a significant contribution to the electron spectral function. The later contribution is peaked below the Fermi level and keeps a pseudogap-like shape. The result of the two contributions to the electron spectral function is a restoration of the particle-hole symmetry in the density of states both in normal and superconducting state at optimal doping. The particle-hole symmetry of the density of states is yet another hint of the proximity to the quantum critical point since it is well known that only this symmetry allows non trivial criticality in the two impurity Kondo model [11].

Transition into the superconducting state: The degeneracy responsible for the strongly incoherent metal with large scattering rate at the Fermi level is lifted by the superconductivity avoiding the quantum critical point. Fig. 4a shows that both important singlet pseudoparticles (for N=4 and N=2) develop a very sharp peak at the same treshold frequency and, at the same time, their occupancy increases (see Fig. 4c) upon condensation, indicating that electrons are locked into singlets with zero momentum. A gap opens between the singlets and doublets which gives the gap in the one-particle density of states. Because of this gap in the pseudoparticle thresholds, the large imaginary part of the electron self-energy does not persist in the superconducting state (see also Fig. 1). Since the density of states is composed of two almost equally important contributions, i.e., the convolution of the doublet with both singlets (N=4 and N=2), the superconducting gap is almost particle hole symmetric in the optimally doped regime with half-width of the order of 0.12t. When the doping value is changed from its critical value, the asymmetry in the superconducting density of states appears. The magnitude of the assymetry is the same as the asymmetry of the corresponding normal state spectra and comes from the fact that the occupancy and therefore importance of the N=4 half-filled singlet exceeds the importance of the N=2 singlet (see Fig. 4c). The spin susceptibility comes almost entirely from the convolution of the half-filled singlet with the half-filled triplet ($N = 4, S = 1, K = (\pi, \pi)$). The later develops a peak at an energy $0.16t$ upon condensation which causes the resonance in the spin susceptibility.

In conclusion we showed that at optimal doping, in the t-J model, there is a collapse of coherence scale, accompanied by a a large scattering rate, restoration of particle-hole symmetry, which result in approximate power laws in physical quantities, such as the optical conductivity ($\sigma \propto \omega^{-2/3}$) and spin susceptibility ($\chi_{\pi\pi} \propto \omega^{-2}$). Quantum criticality is avoided when electrons condense into a supercondacting state which results in a dramatic reduction of scattering rate, the formation of an energy gap which in turns leads to a resonance in the spin susceptibility. A transparent physical interpretation of the numerical results was given in terms of pseudoparticles which represent the important many body excitations, fermionic quasiparticles and bosonic collective modes. This real space picture complements the momentum space picture which emerges in other studies, where substantial deformations of the Fermi surface which result in the formation of Fermi arcs at comparable values of the doping [5, 12]. Finding analytic connection between single particle properties in k space and the collective excitations presented in this study is an interesting direction for future research.

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